4,7,10,13,16,19-Docosahexaenoic acid, methyl ester, (all-Z)-

Other names: (all-Z)-Methyl Docosa-4,7,10,13,16,19-hexaenoate
Z,Z,Z,Z,Z,Z 4,7,10,13,16,19-docosahexaeneoate
cis-4,7,10,13,16,19-Docosahexaenoic acid, methyl ester
methyl Z,Z,Z,Z,Z,Z 4,7,10,13,16,19-docosahexaeneoate

Inchi: InChI=1S/C23H34O2/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23(24)2

InchiKey: VCDLWFYODNTQOT-JDPCYWKWSA-N

Formula: C23H34O2

SMILES: CCC=CCC=CCC=CCC=CCC=CCC=CCCC(=O)OC

Mol. weight [g/mol]: 342.51

CAS: 2566-90-7

Physical Properties

Property code	Value	Unit	Source
gf	390.18	kJ/mol	Joback Method
hf	-59.53	kJ/mol	Joback Method
hfus	59.32	kJ/mol	Joback Method
hvap	131.80 ± 0.20	kJ/mol	NIST Webbook
log10ws	-7.43		Crippen Method
logp	6.637		Crippen Method
mcvol	316.570	ml/mol	McGowan Method
pc	1062.40	kPa	Joback Method
rinpol	2470.70		NIST Webbook
tb	826.89	K	Joback Method
tc	1023.30	K	Joback Method
tf	390.65	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	942.27	J/mol×K	826.89	Joback Method
cpg	960.24	J/mol×K	859.62	Joback Method
cpg	977.45	J/mol×K	892.36	Joback Method
cpg	994.00	J/mol×K	925.09	Joback Method

cpg	1010.00	J/mol×K	957.83	Joback Method
cpg	1025.54	J/mol×K	990.56	Joback Method
cpg	1040.72	J/mol×K	1023.30	Joback Method
dvisc	0.0008093	Pa×s	390.65	Joback Method
dvisc	0.0002734	Pa×s	463.36	Joback Method
dvisc	0.0001240	Pa×s	536.06	Joback Method
dvisc	0.0000679	Pa×s	608.77	Joback Method
dvisc	0.0000423	Pa×s	681.48	Joback Method
dvisc	0.0000289	Pa×s	754.18	Joback Method
dvisc	0.0000211	Pa×s	826.89	Joback Method
hvapt	131.80	kJ/mol	298.15	the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

the vaporization enthaplies and vapor pressures of a series of unstaurated fatty acid methyl esters by correlation gas chromatography: https://www.doi.org/10.1016/j.tca.2007.02.008

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2566907&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume